High-pressure synchrotron X-ray diffraction studies of potassium and complex carbonates

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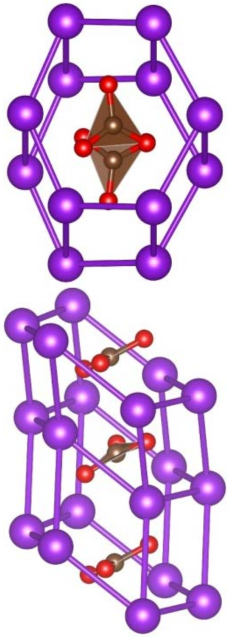
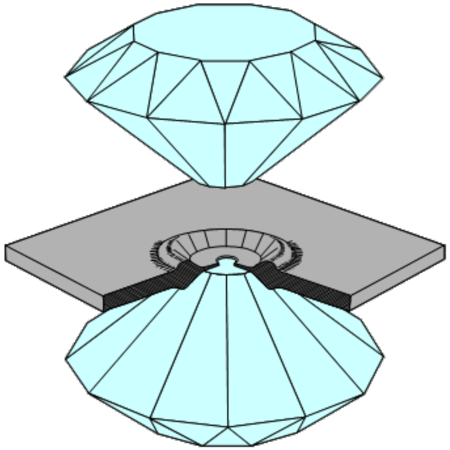
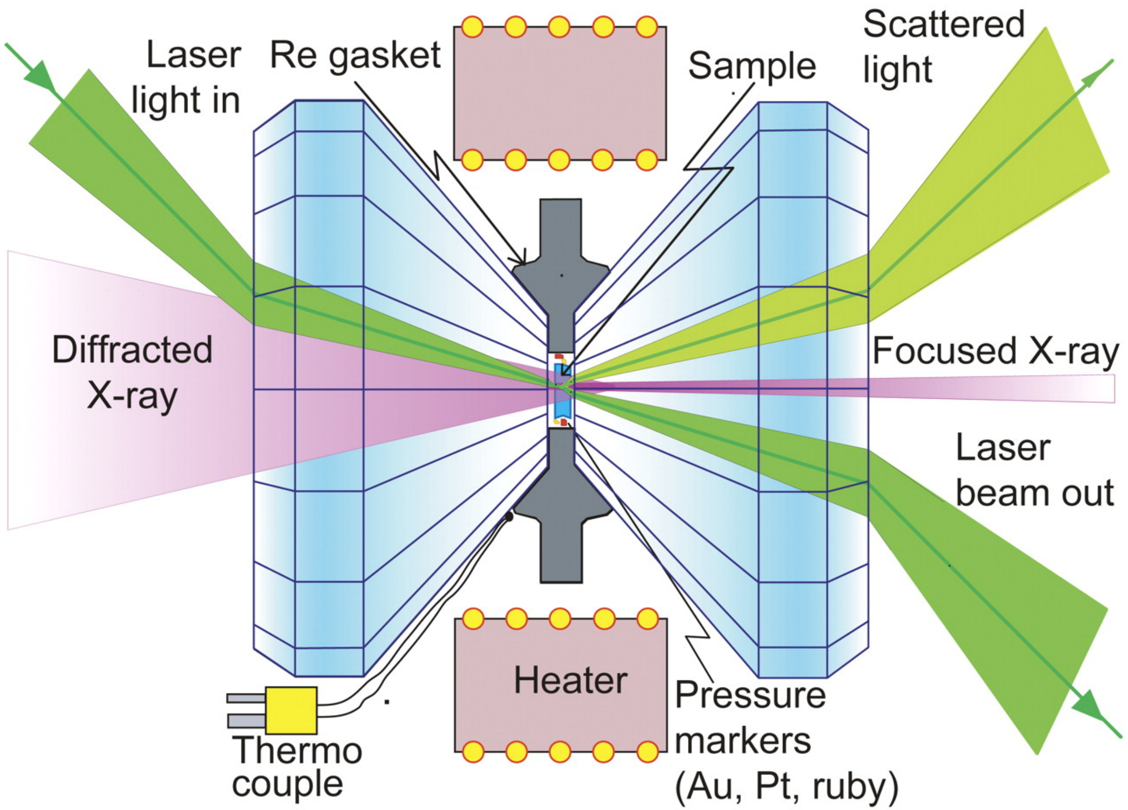
SFR-2016

P2$_1$/c



Diamond-anvil cell technique for high static pressure generation





750 GPa / 6000 K

Matter under extreme conditions: PHYSICS

LETTER

doi:10.1038/nature14964

Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov[1]*, M. I. Eremets[1]*, I. A. Troyan[1], V. Ksenofontov[2] & S. I. Shylin[2]

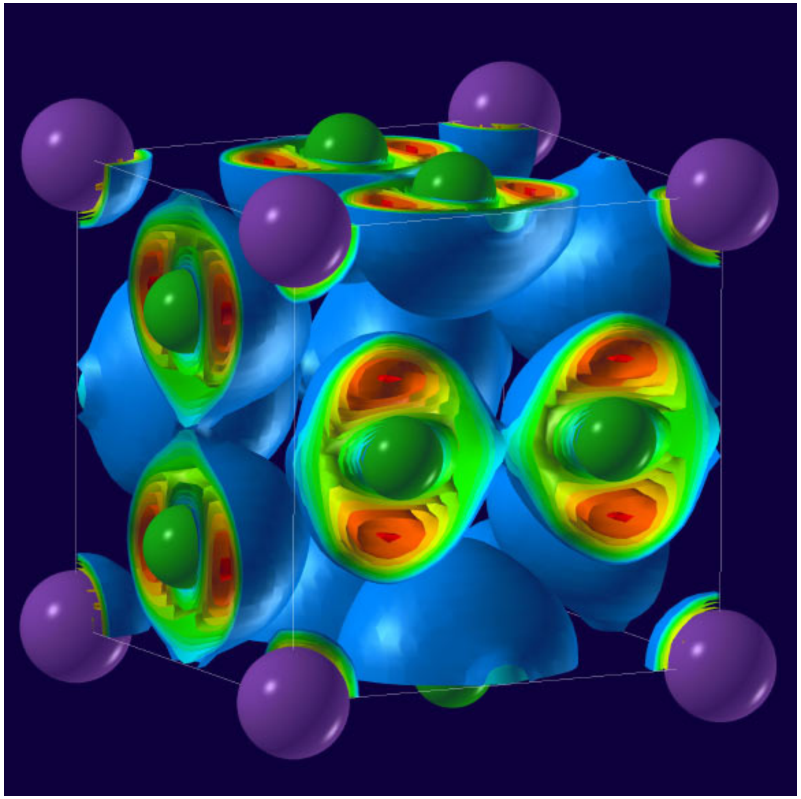
Nature, 2016

Matter under extreme conditions: CHEMISTRY

Unexpected Stable Stoichiometries of Sodium Chlorides

Weiwei Zhang,[1,2*†] Artem R. Oganov,[2,3,4*†] Alexander F. Goncharov,[5,6] Qiang Zhu,[2] Salah Eddine Boulfelfel,[2] Andriy O. Lyakhov,[2] Elissaios Stavrou,[5] Maddury Somayazulu,[5] Vitali B. Prakapenka,[7] Zuzana Konôpková[8]

Science, 2013

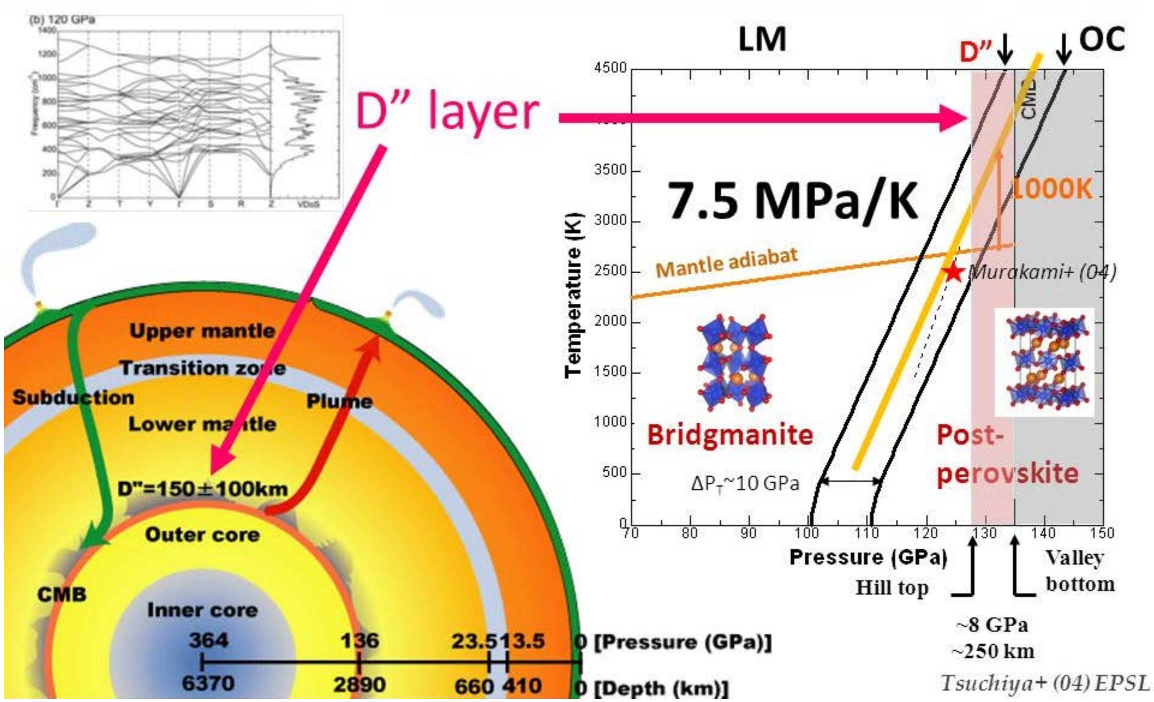


$NaCl_3$ (60 GPa)

Matter under extreme conditions: EARTH SCIENCES

Post-Perovskite Phase Transition in $MgSiO_3$

Motohiko Murakami,[1*] Kei Hirose,[1*] Katsuyuki Kawamura,[1]
Nagayoshi Sata,[2] Yasuo Ohishi[3]



Science, 2004

Matter under extreme conditions: PLANETARY SCIENCES

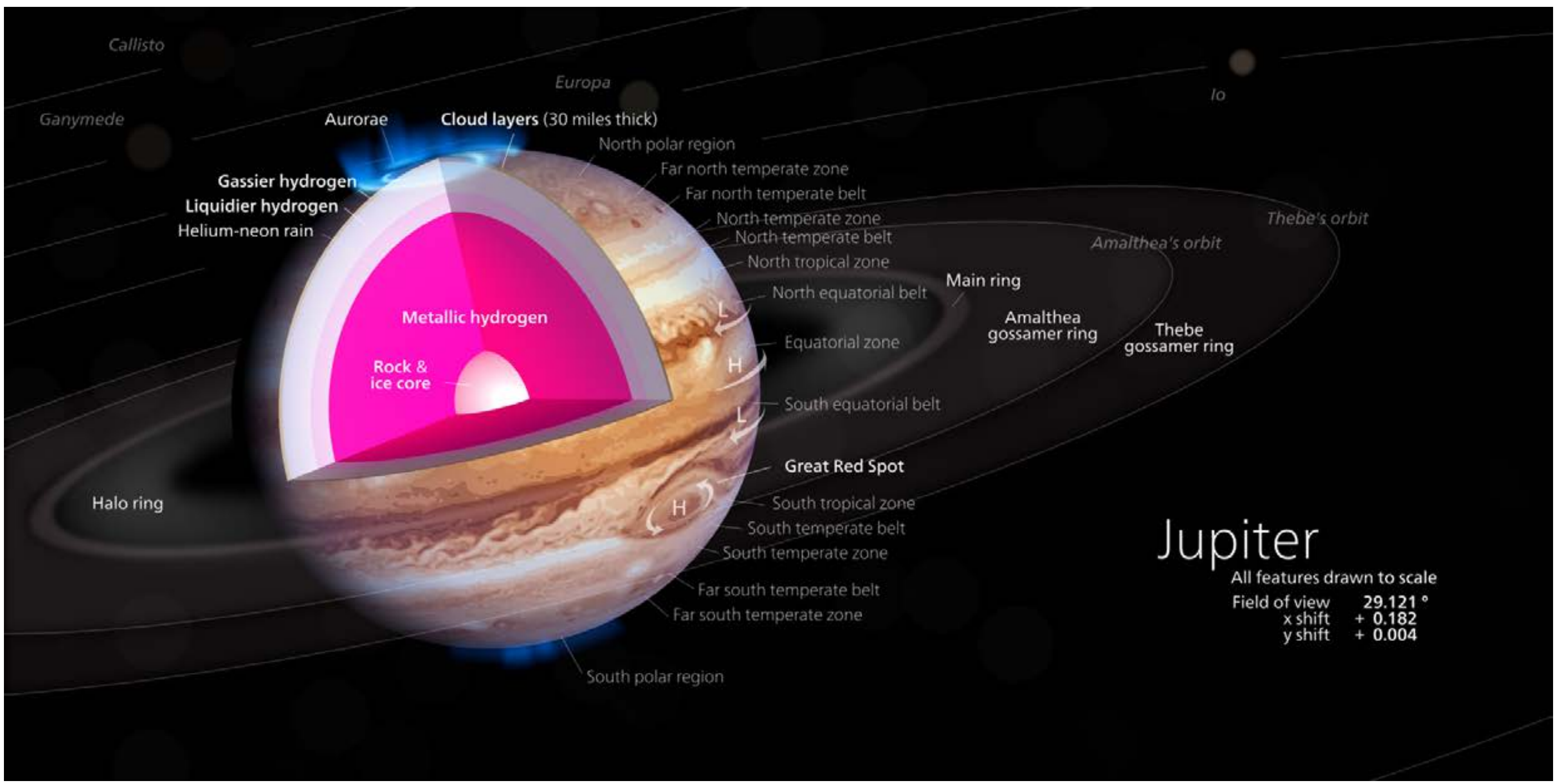
Nature, 2016

LETTER

doi:10.1038/nature16164

Evidence for a new phase of dense hydrogen above 325 gigapascals

Philip Dalladay-Simpson[1], Ross T. Howie[1]† & Eugene Gregoryanz[1,2]



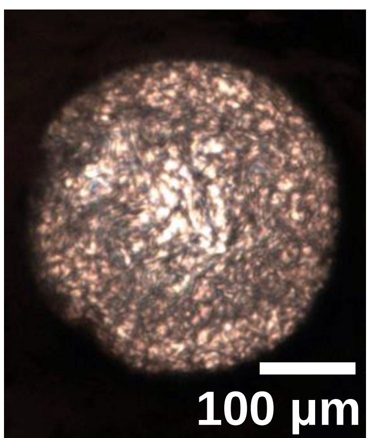
BL04 “Diffractometry in hard X-rays”:

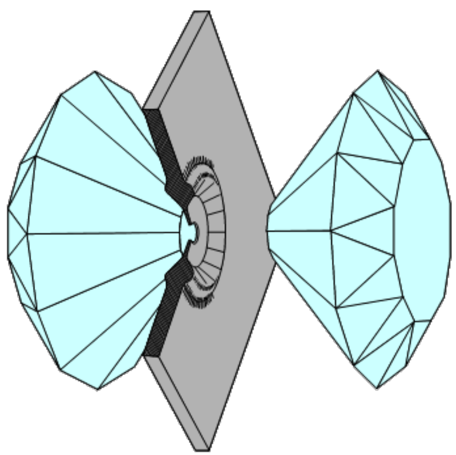
a high-pressure X-ray diffraction beamline at the VEPP-3 storage ring

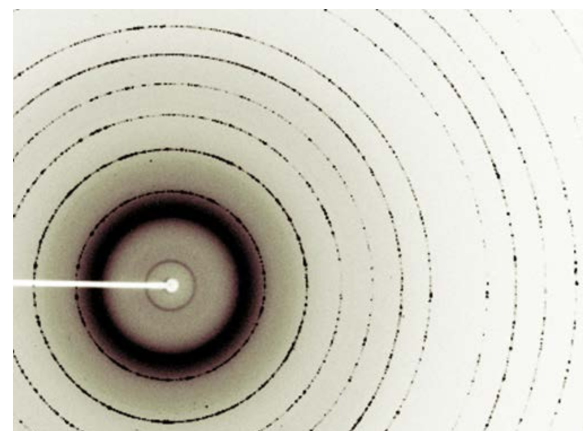
of the Siberian Synchrotron Radiation Centre

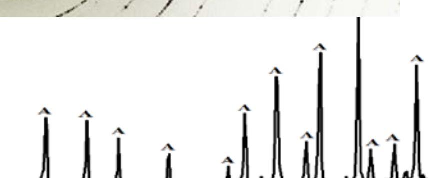
(Budker Institute of Nuclear Physics, Novosibirsk)

- Si (111) monochromator: 33.7 keV / 0.3685 Å (diamond transparency!)
- MAR345 image plate detector (34.5 cm in diameter)
- Unit cell and Rietveld structure refinement of materials under extreme conditions

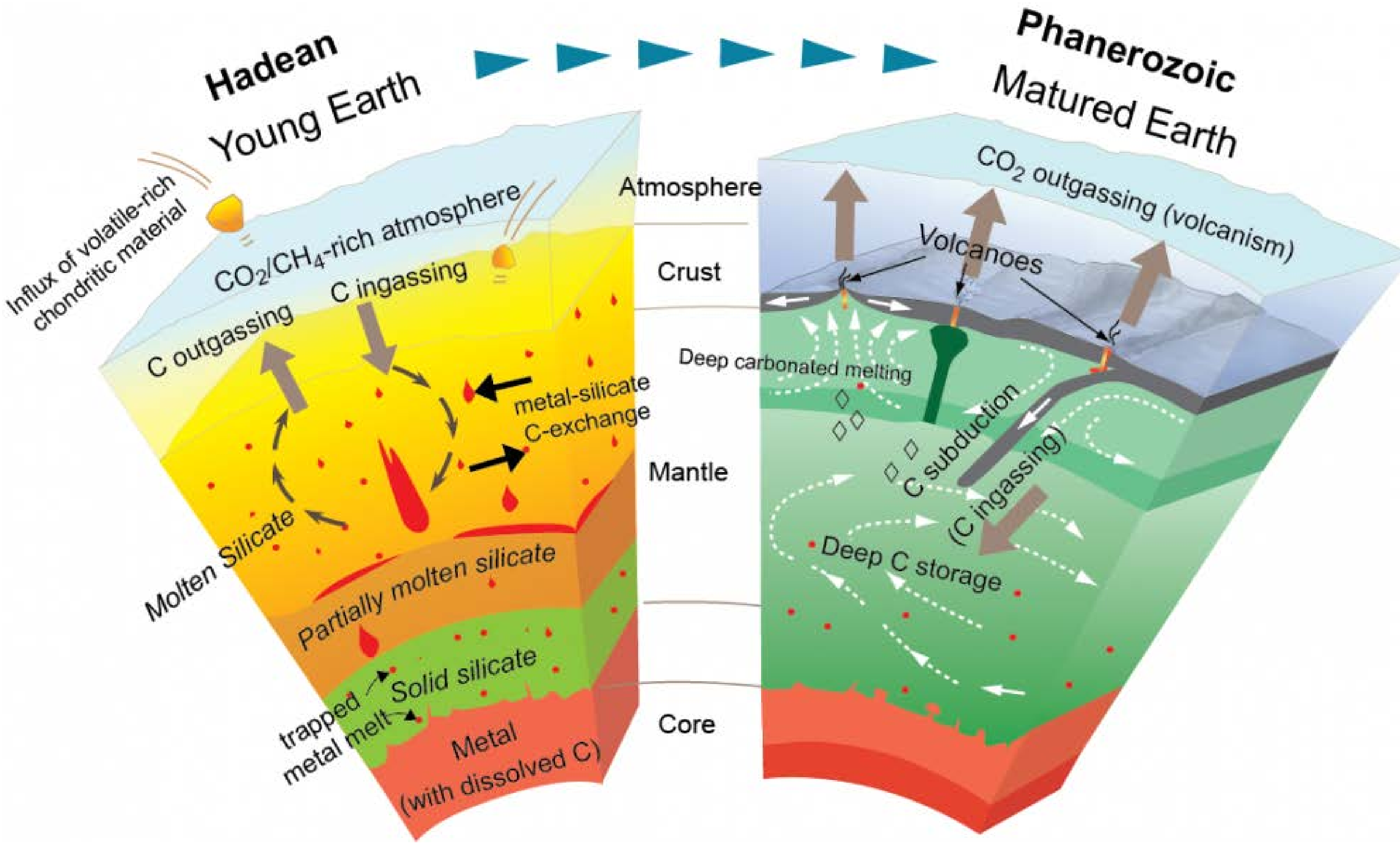






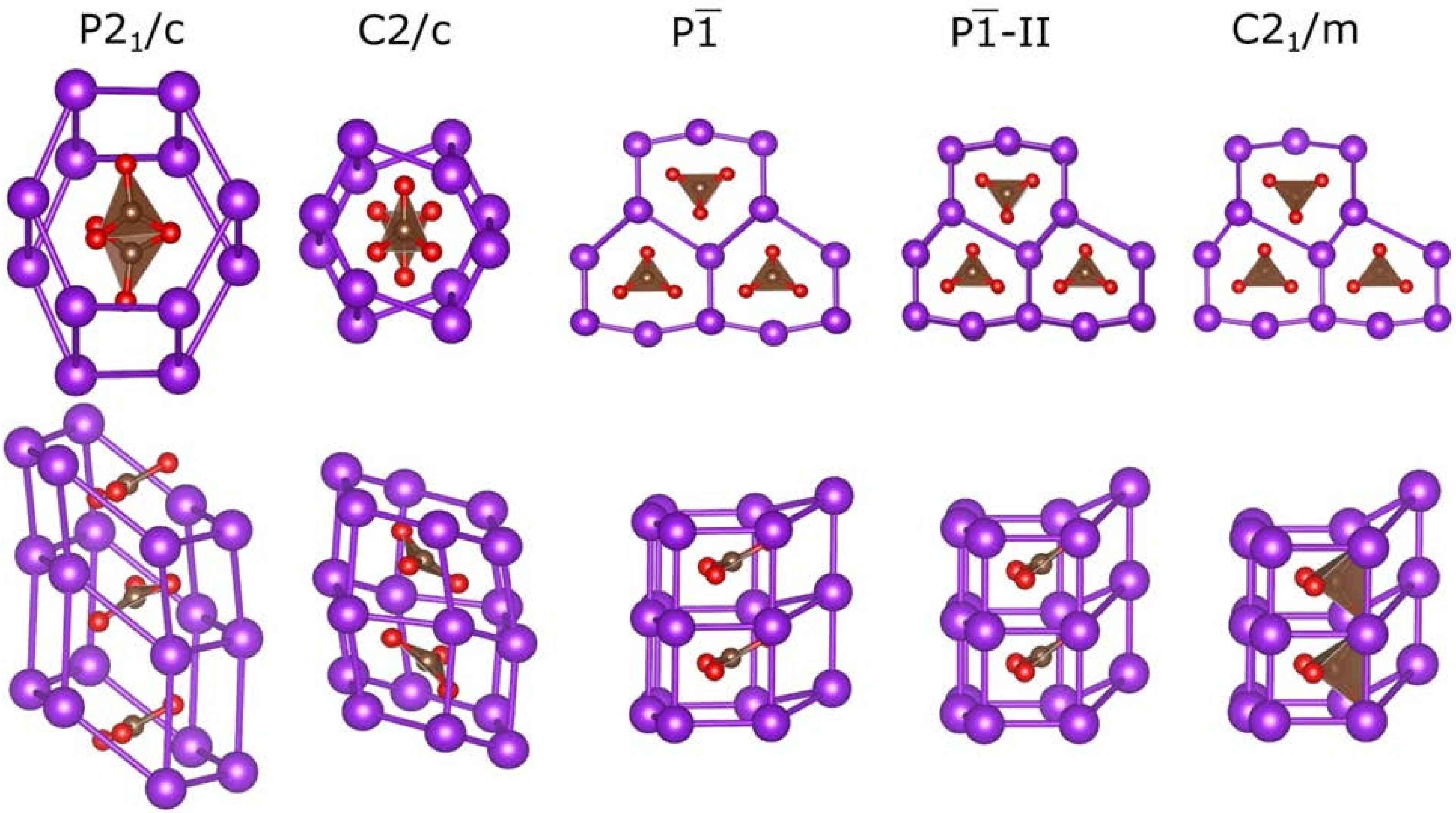


High-pressure studies of geomaterials: alkali and complex carbonates



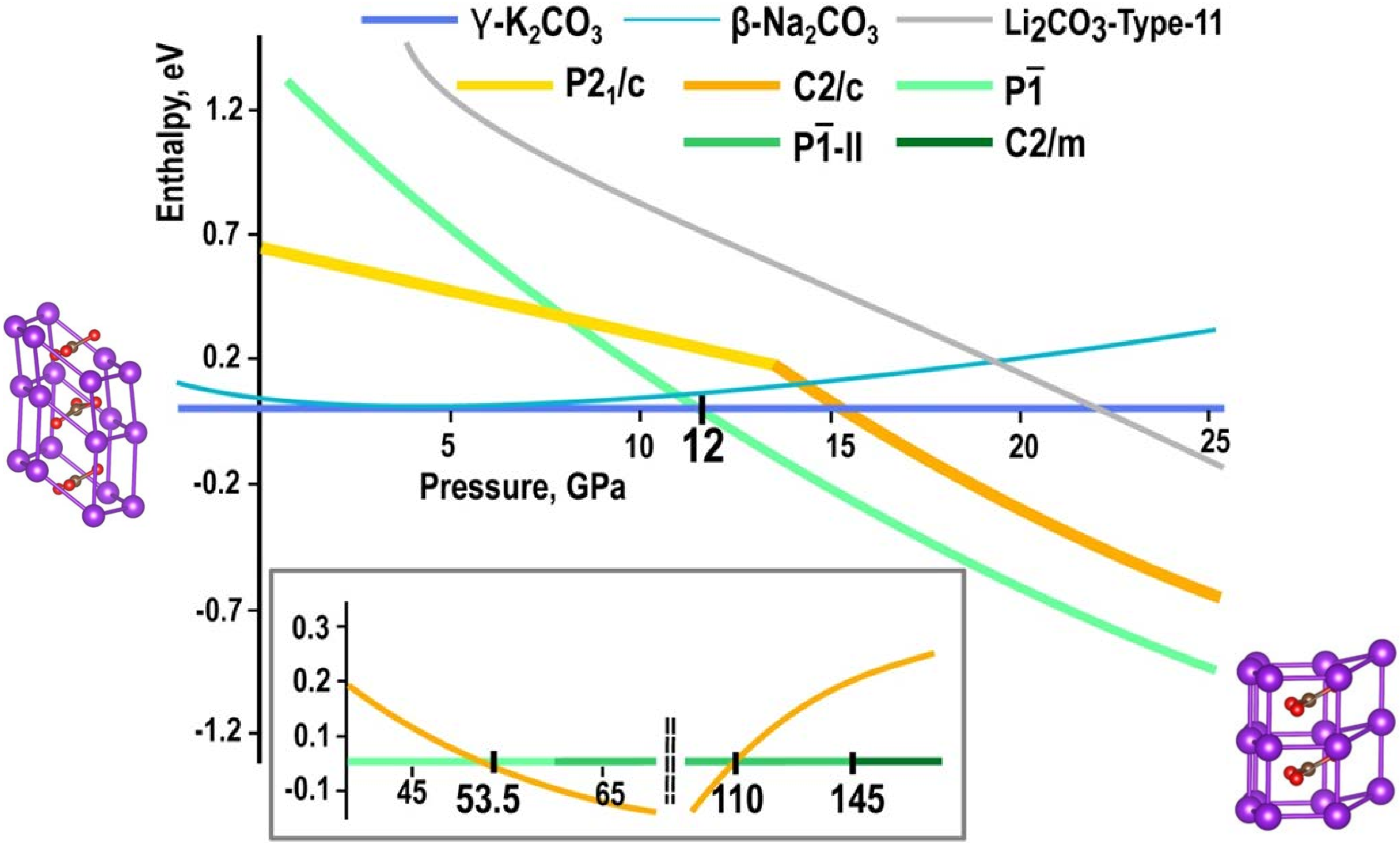
Deep carbon cycle

I. High-pressure phases of potassium carbonate K_2CO_3: *ab initio* quantum modeling



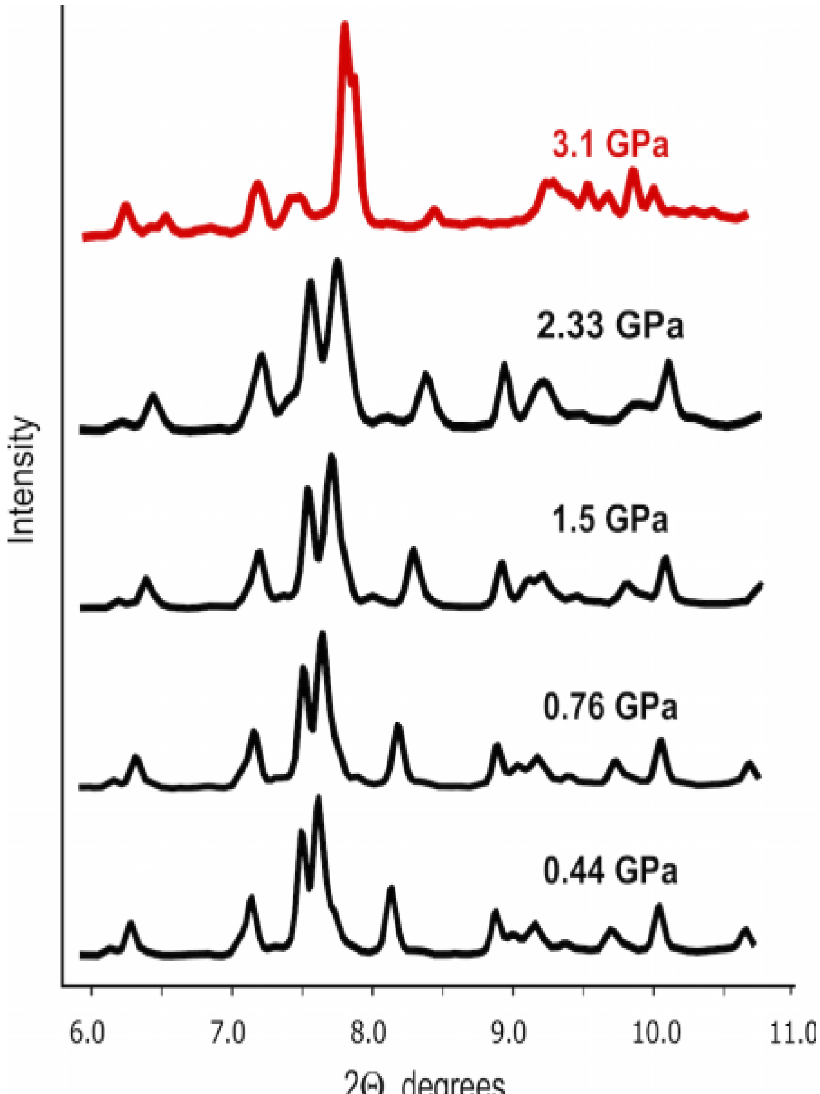
Search of structures by USPEX evolutionary algorithm

I. High-pressure phases of potassium carbonate K_2CO_3: *ab initio* quantum modeling



Energy minimization

I. High-pressure phases of potassium carbonate K_2CO_3: *in situ* synchrotron X-ray diffraction



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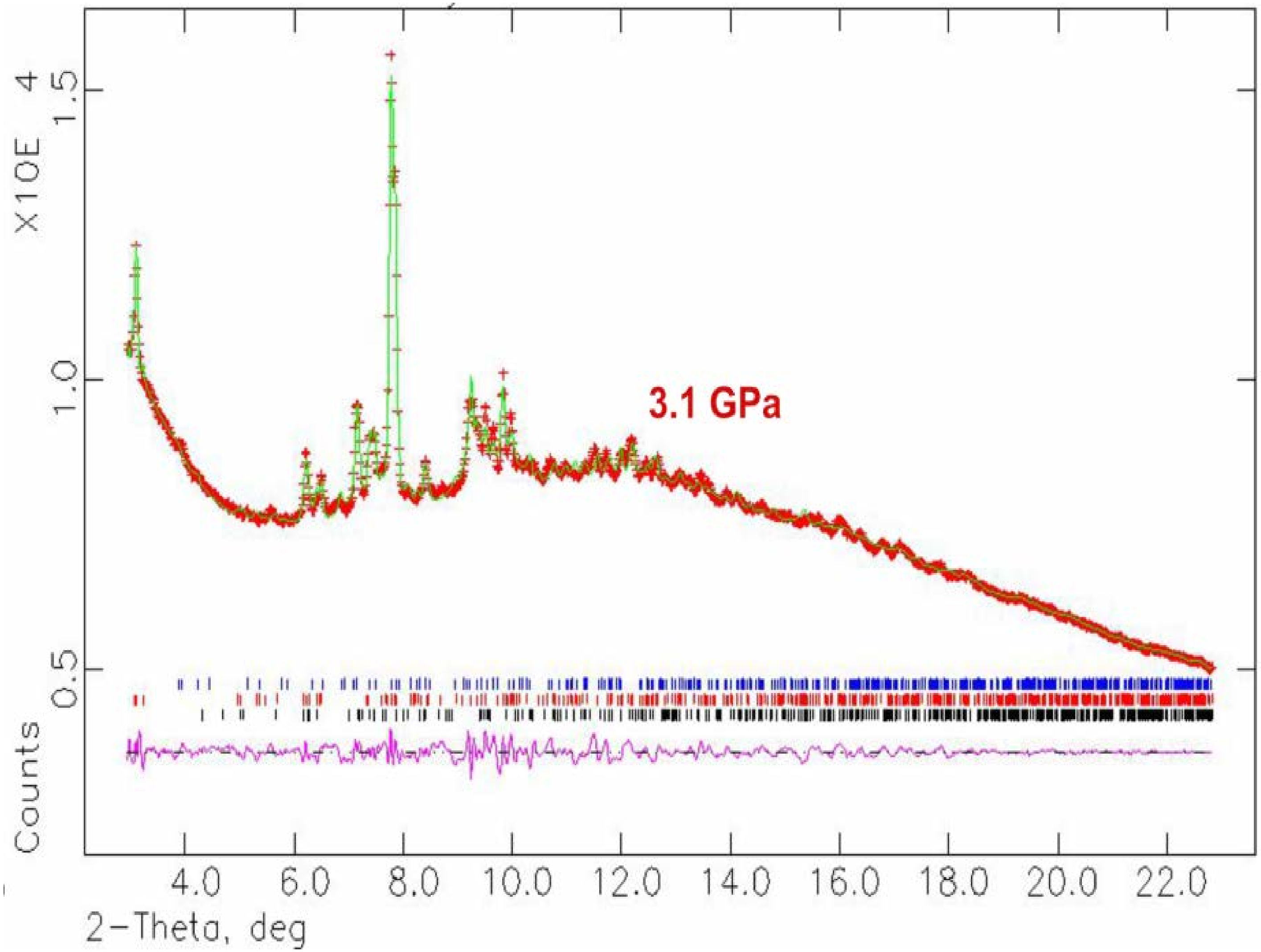
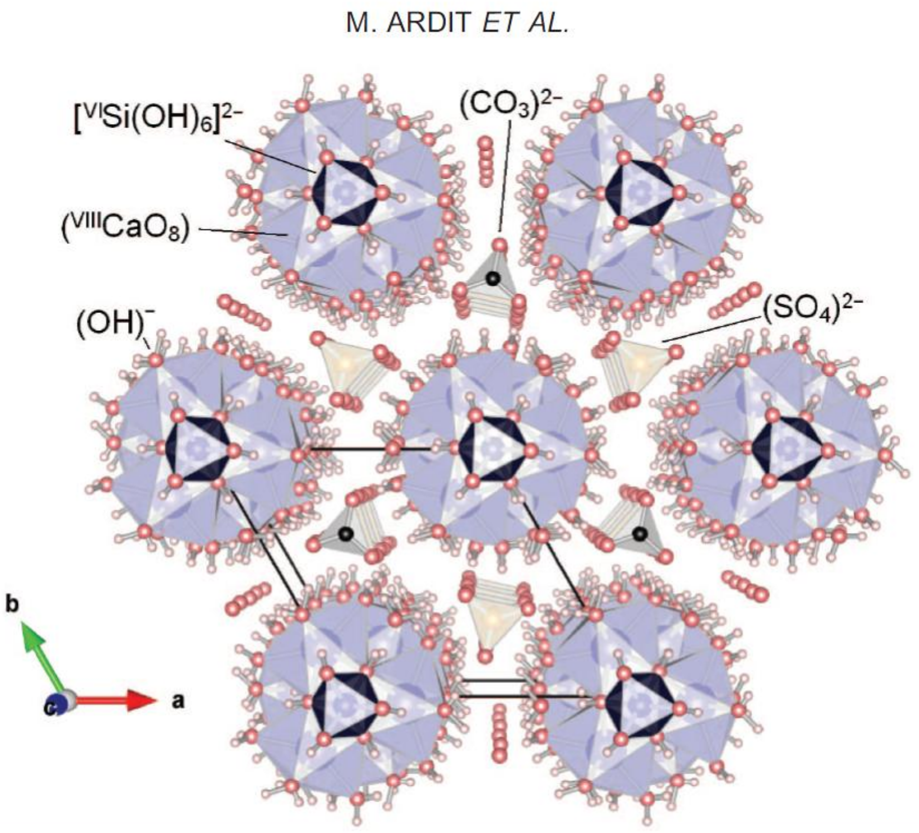


Rietveld refinement: theoretical *P*-1 structure (blue), γ-K_2CO_3 (black), and $K_2CO_3 \cdot 1.5H_2O$ (red)

II. High-pressure study of complex carbonate mineral *thaumasite*, $Ca_3Si(OH)_6(CO_3)(SO_4)\cdot 12H_2O$



Unique crystal chemistry:

- combination of carbonate, sulfate, and $[Si(OH)_6]^{2-}$ anions
- extensive H-bonding net

From Greek *'thaumazein' (to be surprised)*

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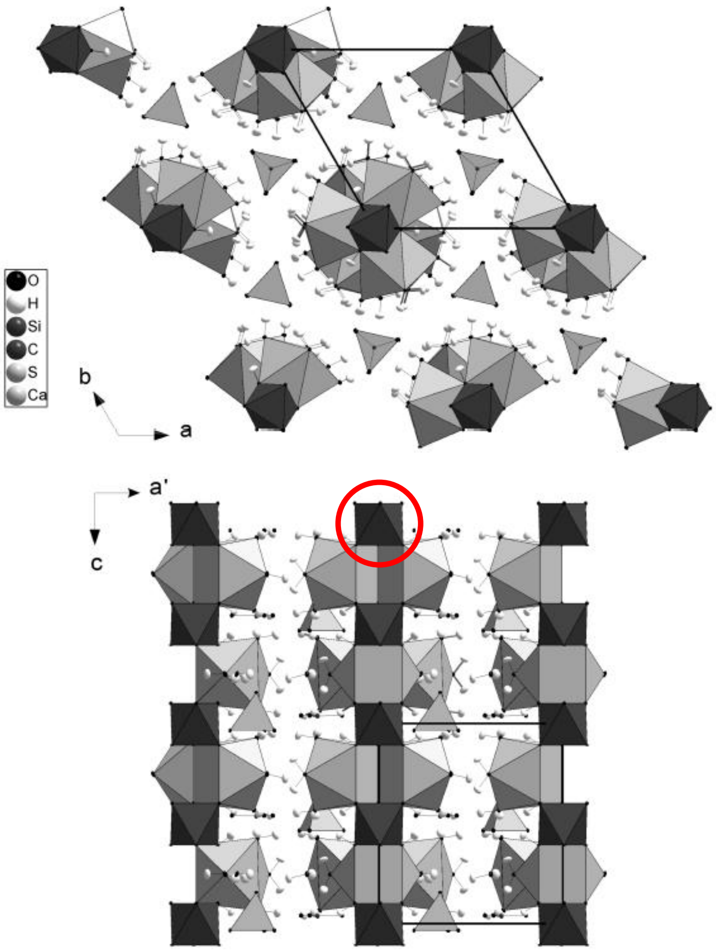


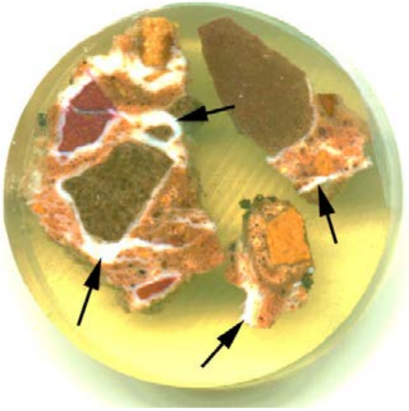
P6 $_3$

a = 11.056 Å, c = 10.414 Å, V = 1102.5 $Å^3$

$[Si(OH)_6]^{2-}$ octahedral anions – an extreme pressure feature:

- 'Phase D' $MgSi_2(OH)_2O_4$ (P > 30 GPa)
- Hydroxide perovskite $MgSi(OH)_6$ (P > 10 GPa)

Thaumasite sulfate attack (TSA)



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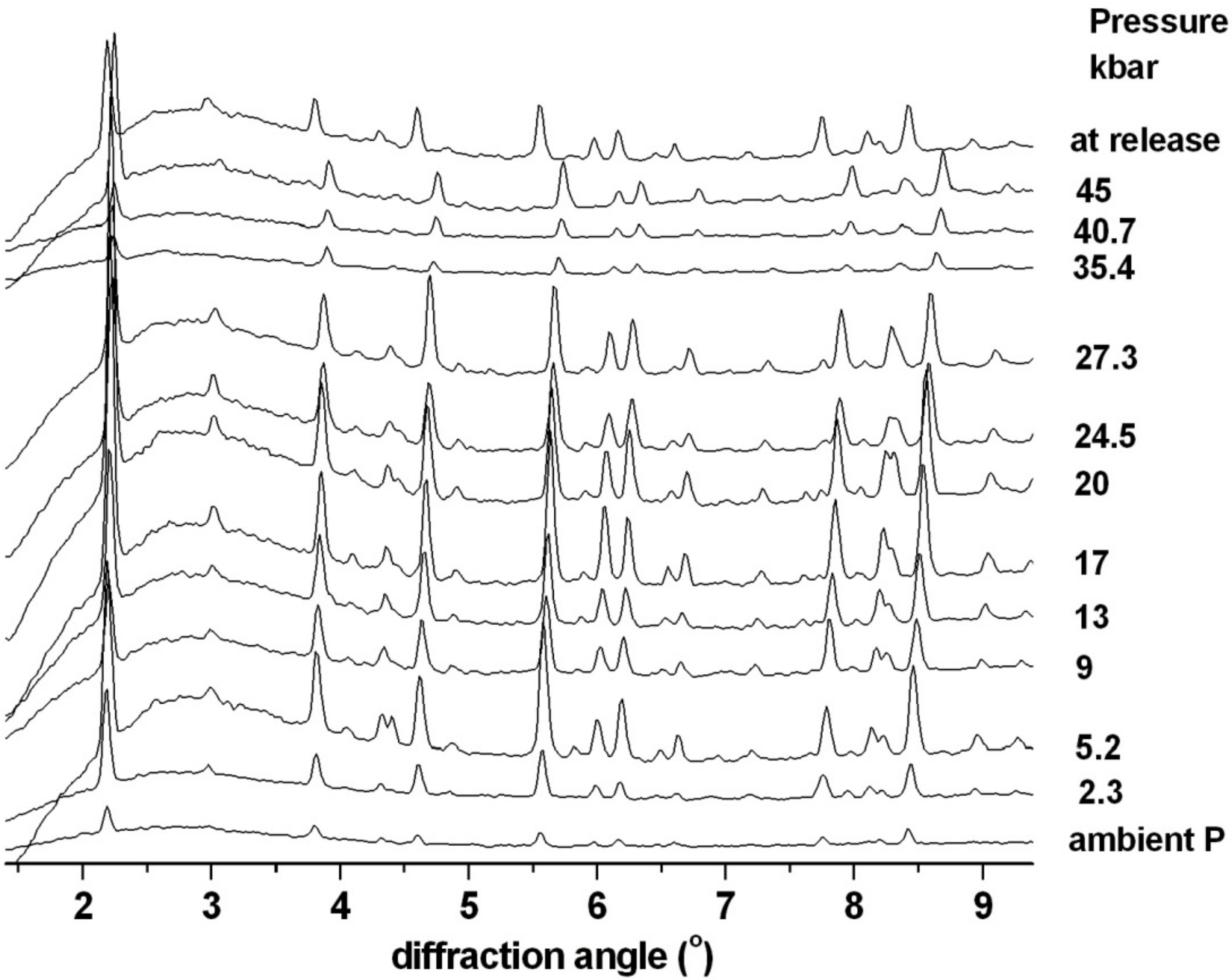

Diffraction patterns of thaumasite compressed in methanol : ethanol : H_2O (quasi)hydrostatic pressure medium (16:3:1 vol.)

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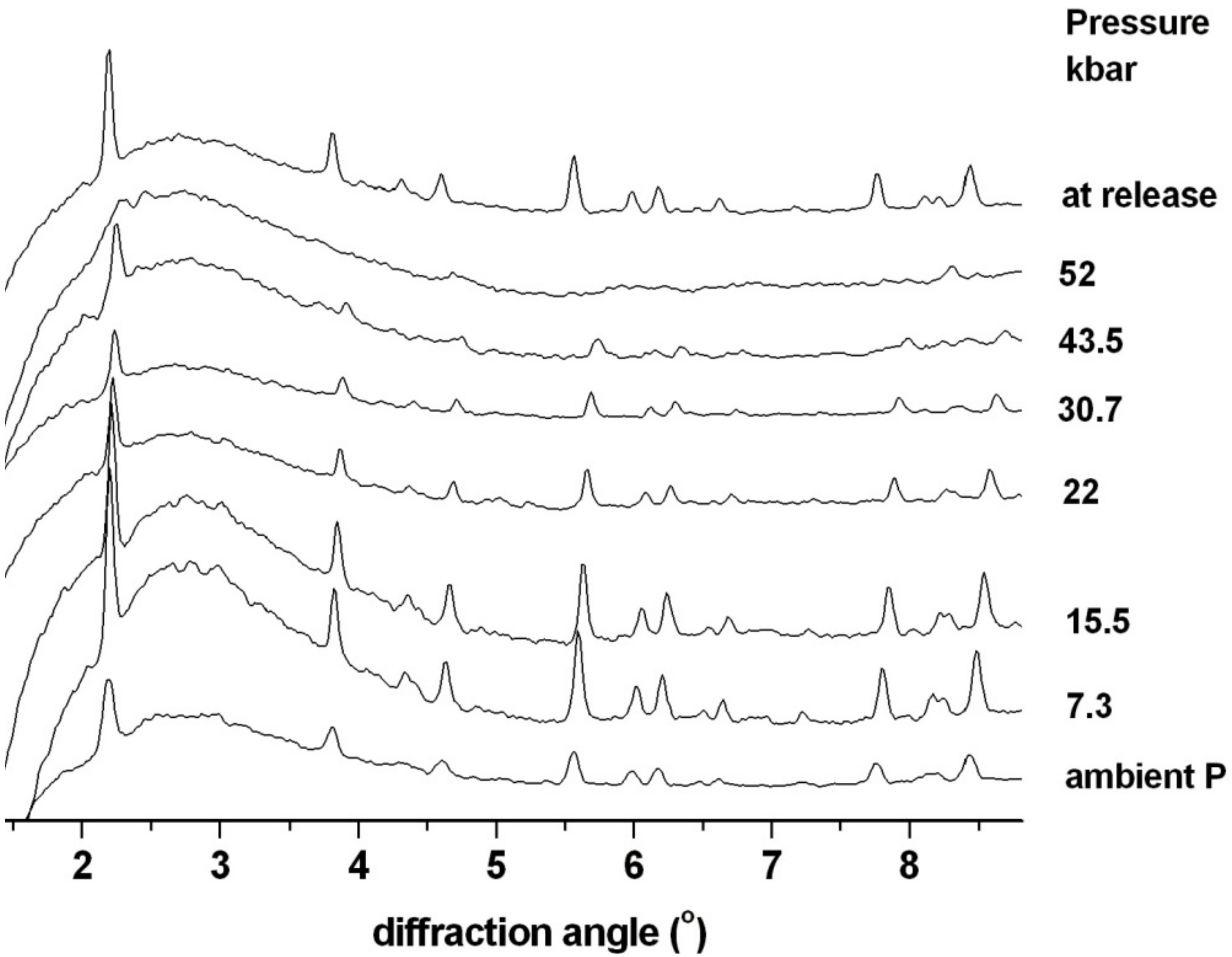

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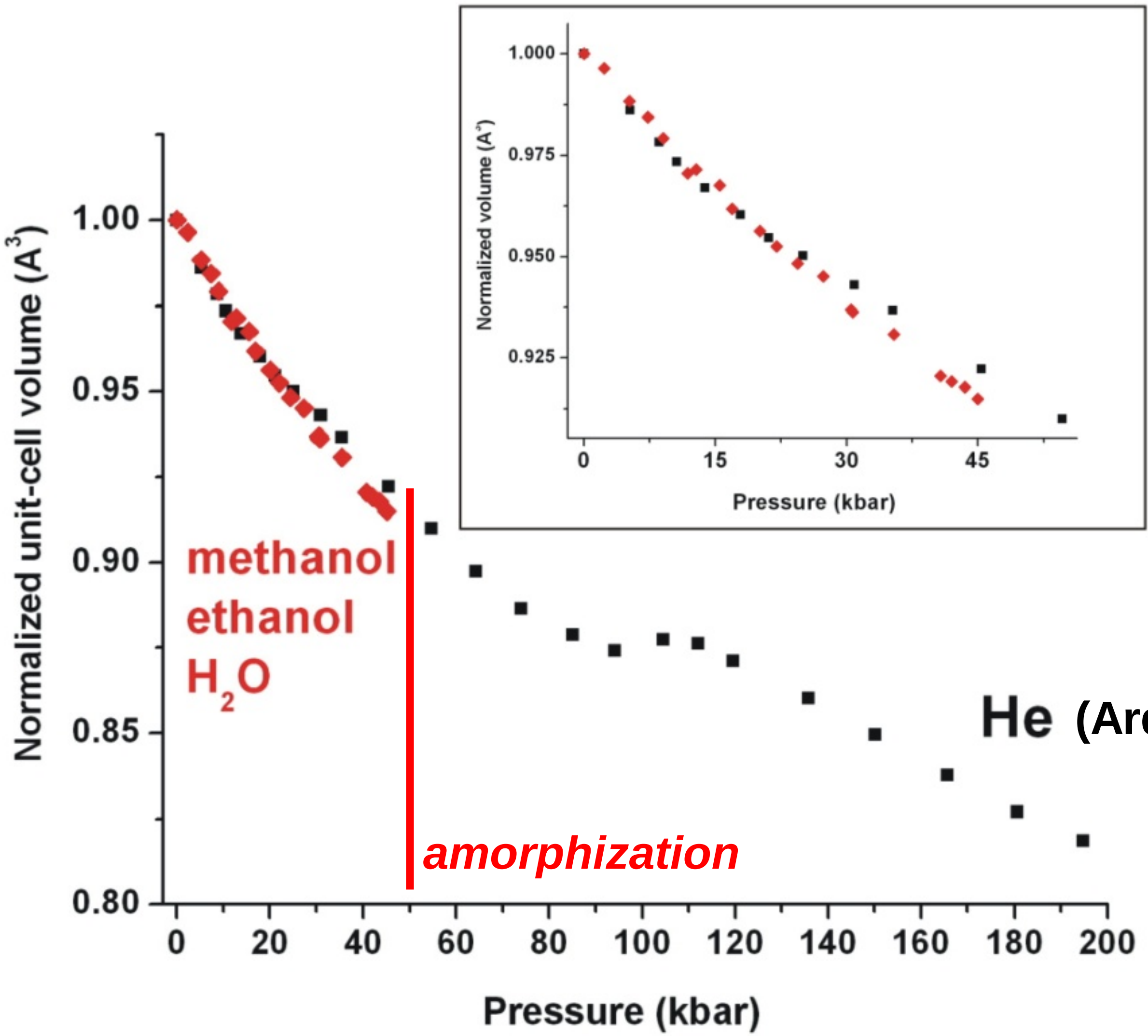

(Ardit *et al.*, 2014, *Min. Mag.*)

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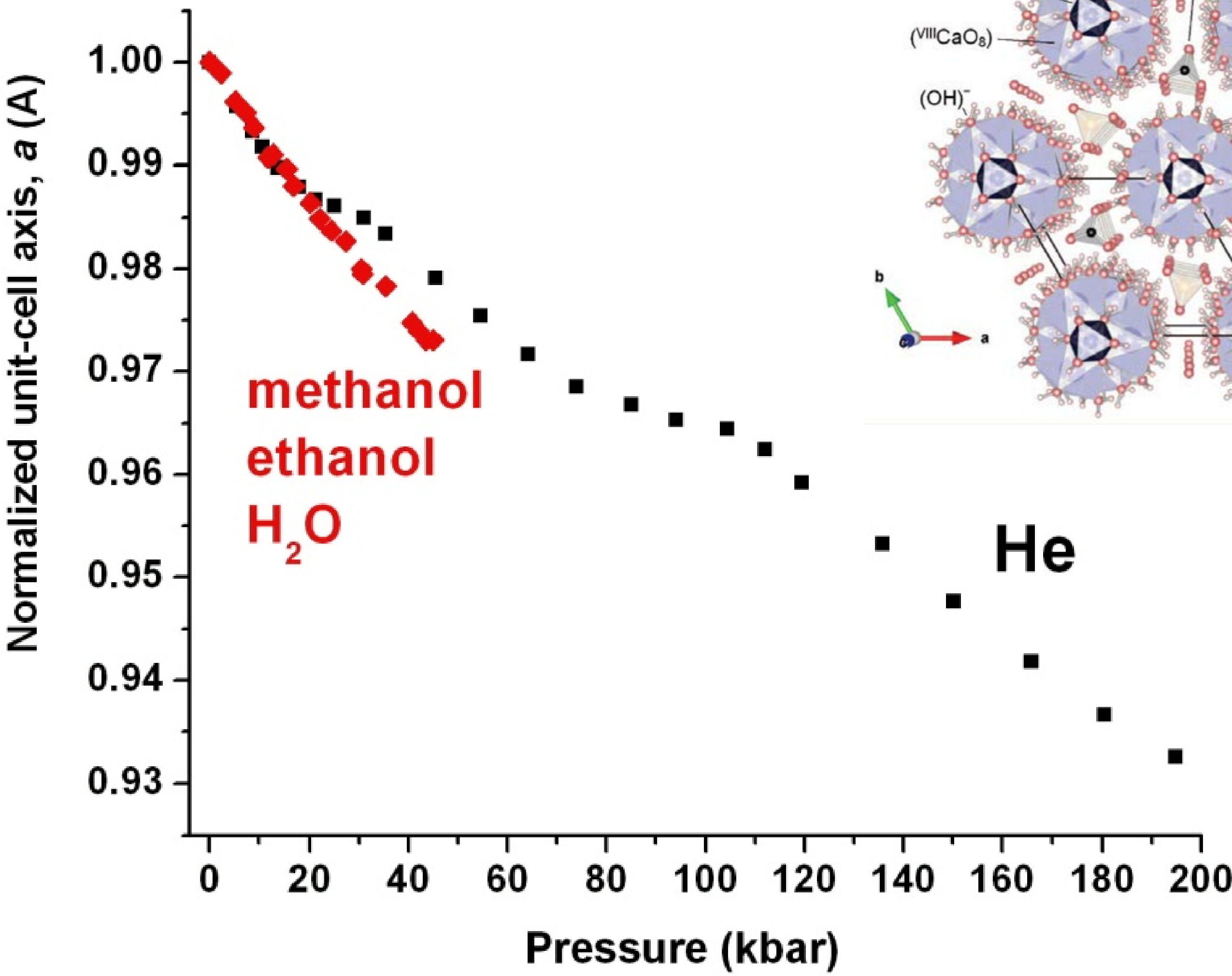
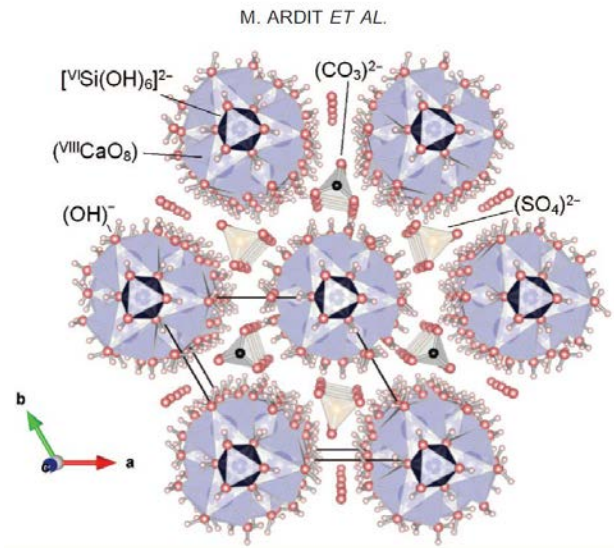




PNAS

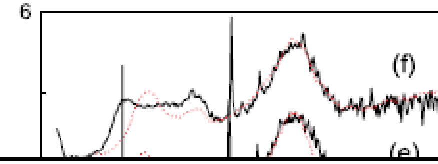
Effect of helium on structure and compression behavior of SiO_2 glass

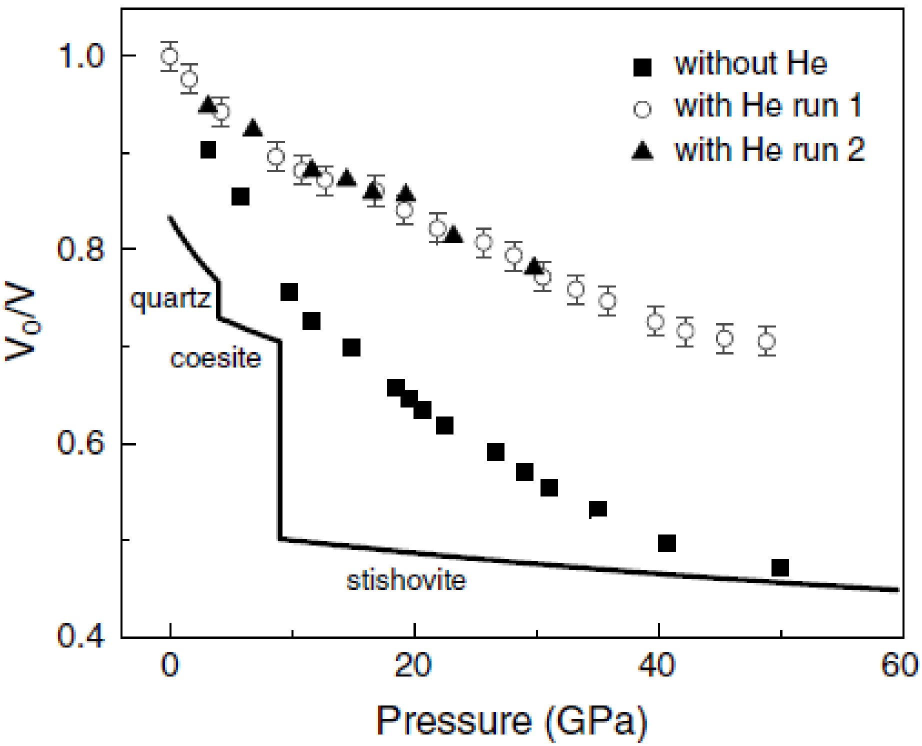
Guoyin Shen[a,1], Qiang Mei[a], Vitali B. Prakapenka[b], Peter Lazor[c], Stanislav Sinogeikin[a], Yue Meng[a], and Changyong Park[a]

[a]High Pressure Collaborative Access Team, Geophysical Laboratory, Carnegie Institution of Washington, Argonne, IL 60439; [b]Center for Advanced Radiation Sources, University of Chicago, Chicago, IL 60637; and [c]Department of Earth Sciences, Uppsala University, 75236 Uppsala, Sweden

Edited by Alexandra Navrotsky, University of California, Davis, CA, and approved March 2, 2011 (received for review February 14, 2011)

The behavior of volatiles is crucial for understanding the evolution of the Earth's interior, hydrosphere, and atmosphere. Noble gases as neutral species can serve as probes and be used for examining gas solubility in silicate melts and structural responses to any gas inclusion. Here, we report experimental results that reveal a strong





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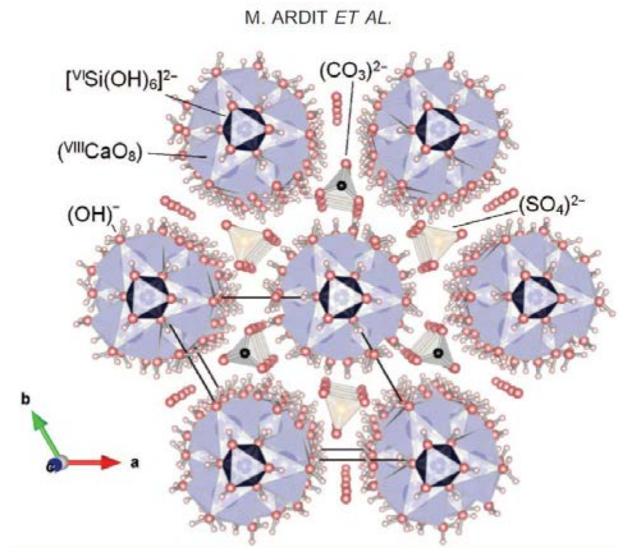

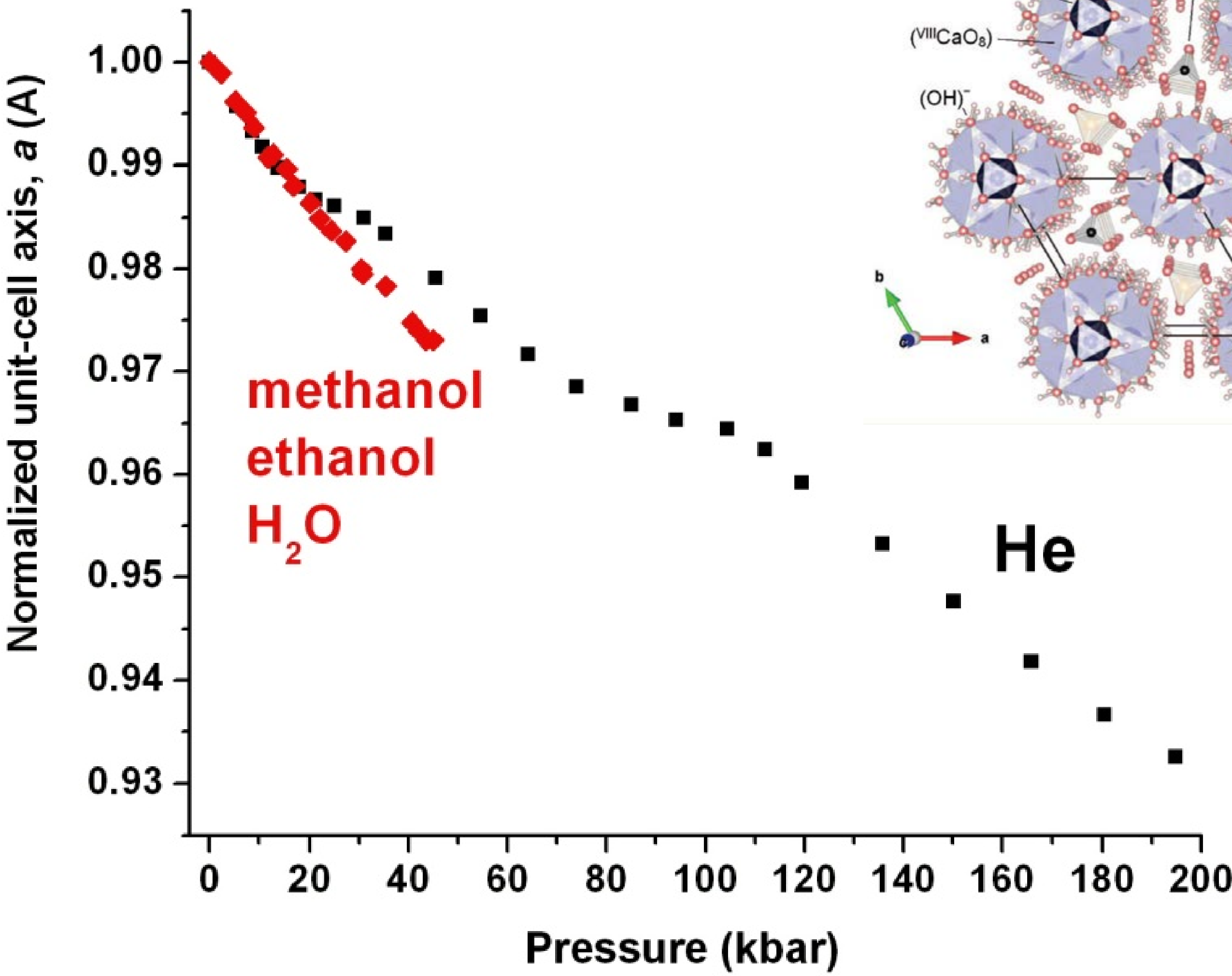

Conclusions

- A high pressure *P*-1 structure predicted for K_2CO_3 from *ab initio* calculations was experimentally confirmed (but at lower *P*)

- No phase transitions were observed in *thaumasite* under R*T* compression up to amorphization above 5 GPa

- Helium is not *an inert*, but ***a penetrating*** medium for thaumasite-like compounds

- Pressure-induced penetration of He into thaumasite structure stabilizes it against amorphization

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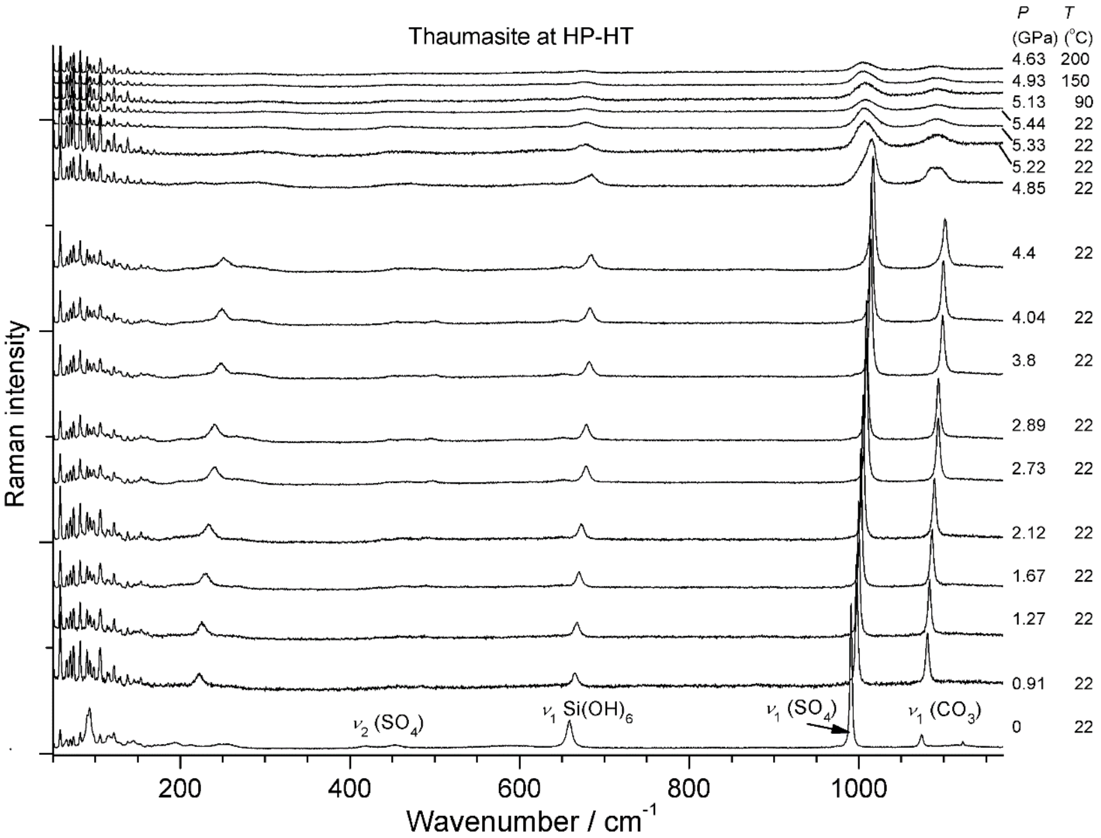
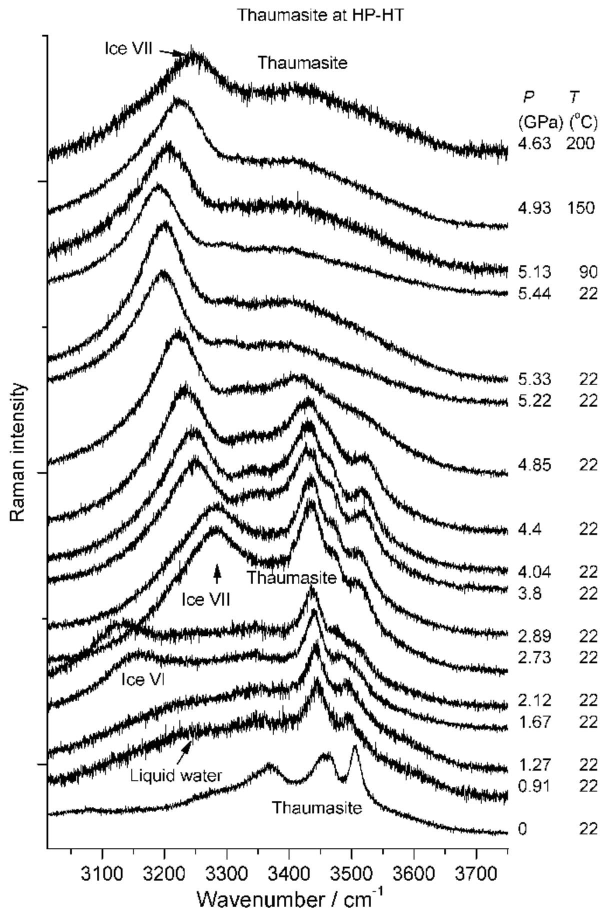
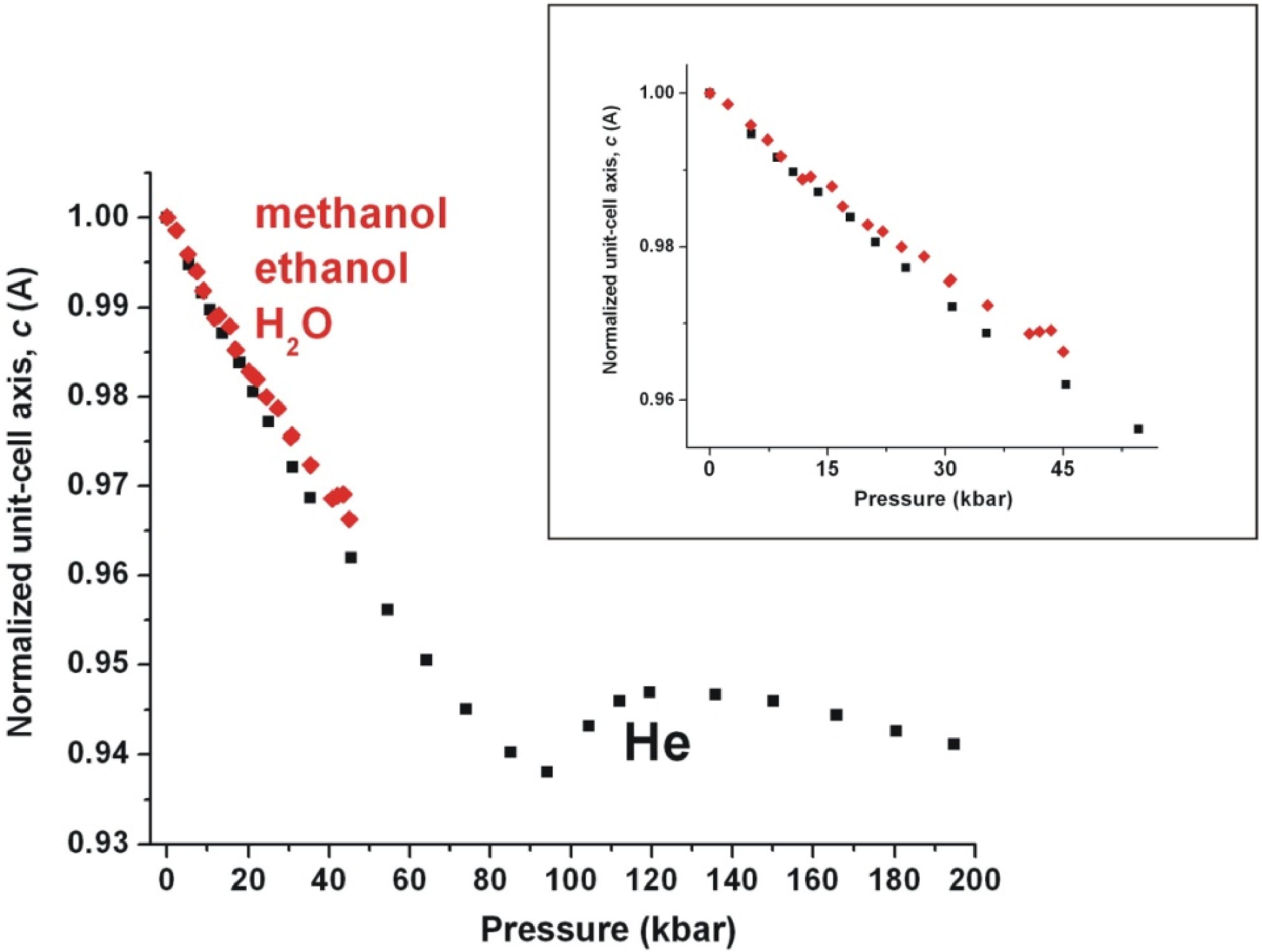
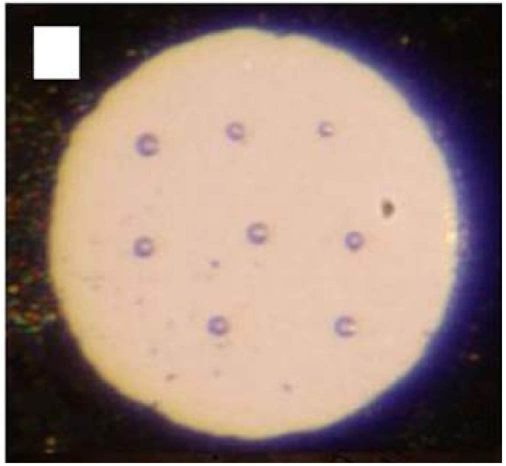
Raman spectra of thaumasite at high pressure

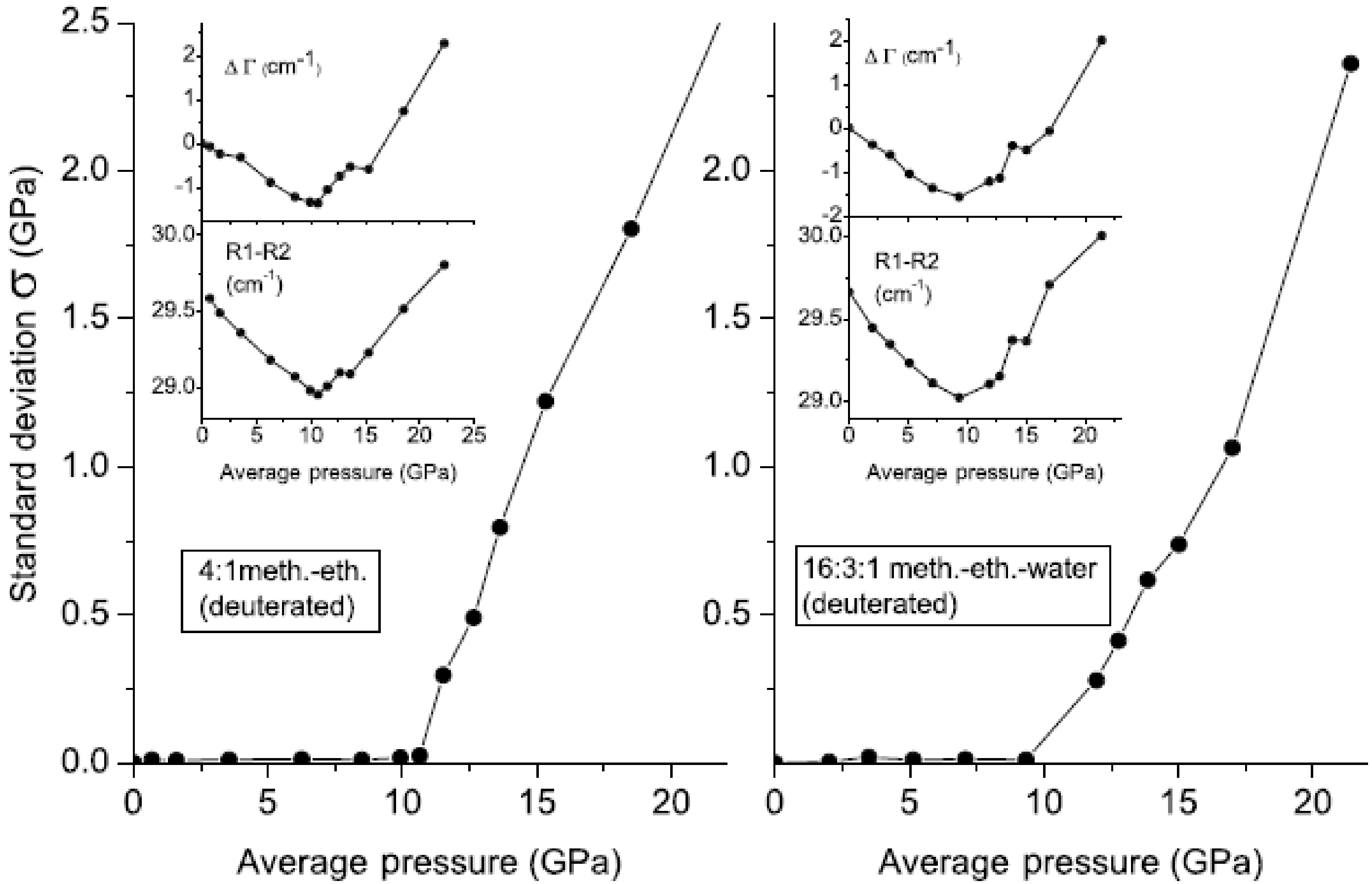






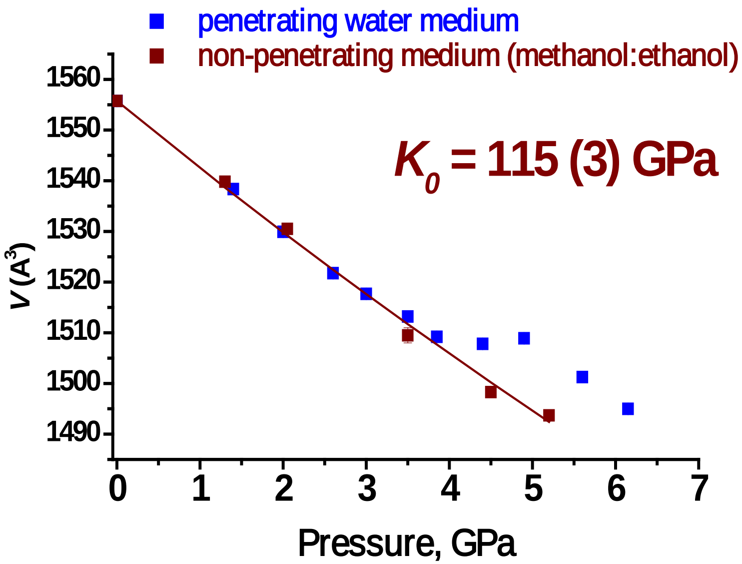
methanol
ethanol
H_2O
He
Normalized unit-cell axis, c (A)
Pressure (kbar)
1.00
0.99
0.98
0.97
0.96
0.95
0.94
0.93
0 20 40 60 80 100 120 140 160 180 200
0 15 30 45

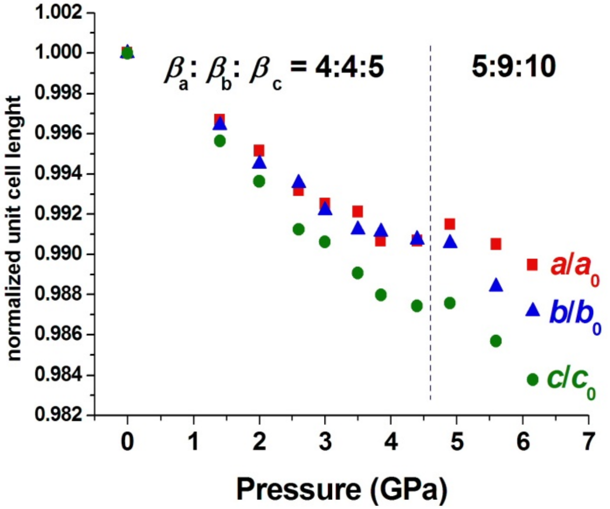




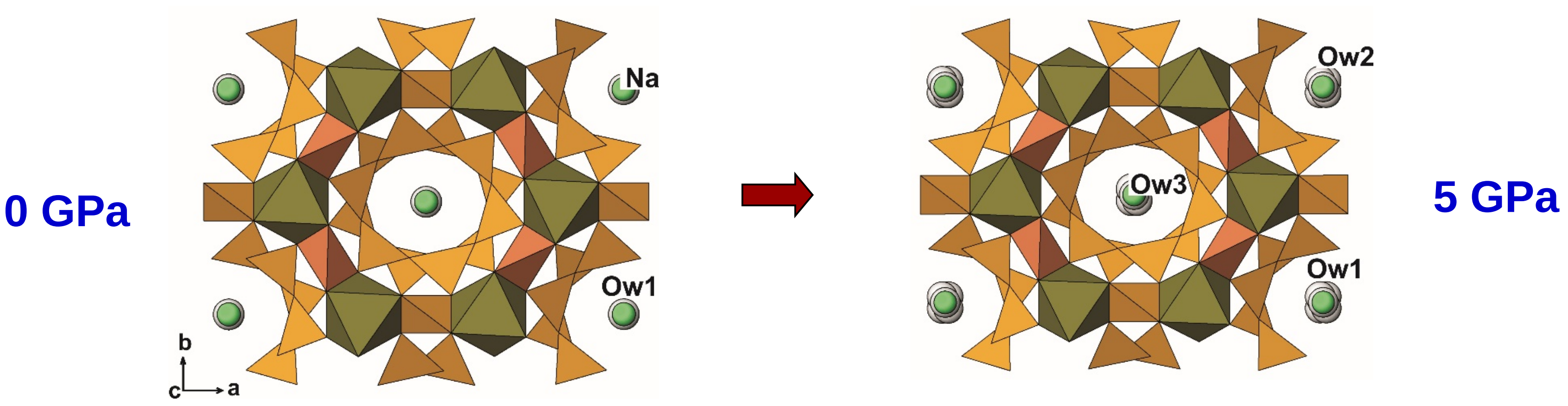
Standard deviation σ (GPa)
Average pressure (GPa)
4:1meth.-eth.
(deuterated)
16:3:1 meth.-eth.-water
(deuterated)
Δ Γ (cm-1)
R1-R2
(cm-1)

Structural transformation in natural cordierite at 4.5 GPa, associated with pressure-induced excess hydration





Pressure dependences of the volume and lattice parameters of cordierite (*Cccm*)



$(Mg,Fe)_2[Al_4Si_5O_{18}]*0.45H_2O \rightarrow 0.72H_2O$